201-14743A

HPV Assessment Report
on
Benzenesulphonic acid
CAS No. 98-11-3

September 12, 2003

Submitted on behalf of the Aromatic Sulfonic Acids Association
1850 M Street, NW, Suite 700, Washington DC 20036

Prepared by NOTOX Safety and Environmental Research B.V.
for submission under the US-HPV Challenge Program

Contents

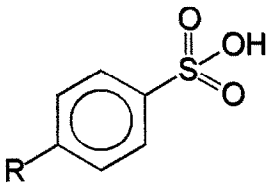
1. Introduction

Capital Resin Corporation, Dynachem, Inc. and Rütgers Organics Corporation formed a consortium known as the Aromatics Sulfonic Acids Association (ASAA) to participate in the United States High Production Volume (HPV) Chemical Challenge Program for benzenesulphonic acid, (CAS 98-11-3). Benzenesulphonic acid is one of several sulphonic acid based industrial chemicals used primarily in the foundry industry as an acid catalyst. Acid catalysts are consumed in the hardening or curing of cold setting polymeric resins used in the preparation of sand molds and cores. The substance is classified as a high production volume (HPV) chemical according to criteria established by the US-EPA, (i.e., > 1,000,000 pounds manufactured or imported into the USA annually). The consortium has agreed to provide all internal documents related to the requirements of the Challenge Program and/or initiate scientifically justified studies for this chemical substance as required to meet the needs of the HPV Chemical Challenge Program.

Under agreement with the consortium, NOTOX Safety and Environmental Research B.V. has conducted an evaluation and assessment of the available data on benzenesulphonic acid (CAS 98-11-3). No data were available from sponsors. For the development of screening health and environmental assessment information, NOTOX examined the public literature. A literature search performed in March 2003 yielded some results. In addition it was examined whether the use of data available from the chemically related substance p-toluenesulphonic acid could fill certain data gaps for benzenesulphonic acid. The rationale for this chemical as a surrogate is described in chapter 2. The suitability of studies retrieved on benzenesulphonic acid and p-toluenesulphonic acid for meeting the SIDS data requirements was determined (summarised in chapter 3), a SIDS data matrix was constructed and recommendations for the draft testing scheme were formulated (data availability analysis; chapter 4). Robust summaries are presented in separate documents as IUCLID data sets.

2. Rationale for the surrogate p-toluenesulphonic acid

For benzenesulphonic acid (CASRN 98-11-3), the closely related substance p-toluenesulphonic acid (CASRN 104-15-4) can be used as a surrogate in view of the chemical similarity between the two compounds (see Figure 1). The extra methyl group para to the sulphonic acid group in p-toluenesulphonic acid has a weakly activating effect on the benzene ring, which makes it slightly more prone to electrophilic aromatic substitution.
Acidity of the sulphonic acid group is influenced by two factors:
1. The methyl group exerts an electron donating effect, which makes the negative charge on the resulting sulphonate ion after deprotonation slightly less stable.
2. The resonance effect still stabilises the negative charge on the sulphonate ion by dividing the charge on the oxygen atoms.
As a result, the acidity of the sulphonic acid group is not expected to change significantly compared to benzenesulphonic acid. Calculation of the pKa confirms this expectation: -2.8 for benzenesulphonic acid and –2.58 for p-toluenesulphonic acid.
Thus the reactivity of benzenesulphonic acid and p-toluenesulphonic acid is very similar and p-toluenesulphonic acid can be used as a surrogate.



CASRN
98-11-3 R=H
104-15-4 R=CH_3

Figure 1. Structure of benzenesulphonic acid (CASRN 98-11-3) and p-toluenesulphonic acid (CASRN 104-15-4).

3. Evaluation of SIDS endpoints

In this chapter an evaluation of data available on SIDS endpoints is given.

Benzenesulphonic acid and p-toluenesulphonic acid are strong acids. In watery environments they are almost completely ionised even at low pH. The typical commercial preparations used as catalysts are 65-70% solutions in water.

3.1. Physico-chemical endpoints

For benzenesulphonic acid data on melting point, boiling point, vapor pressure (calculated), partition coefficient (calculated), water solubility (calculated) and dissociation constant are available. The dissociation constant from the Merck Index and the calculated value differ somewhat, but both indicate that the substance is predominantly ionised in water at neutral pH. The dissociation constant and other physico-chemical properties of p-toluenesulphonic acid are very similar to those of benzenesulphonic acid. The calculated values for vapor pressure are both very low as expected. The calculated values for the partition coefficient indicate that both sulphonic acids dissolve to a much larger extent in water than in octanol as expected from the structural formulas and the dissociation constants indicate that these substances are predominantly ionised in water. The calculated value for water solubility of benzenesulphonic acid is marginally greater than the calculated value of p-toluenesulphonic acid. A lower solubility for p-toluenesulphonic acid may be expected based on the presence of the extra methyl group that renders p-toluenesulphonic acid more hydrophobic, but both sulphonic acids are expected to be highly soluble (>100 grams/liter) in water.

Conclusion: For the physico-chemical endpoints all relevant endpoints are sufficiently investigated and no further testing is warranted.

	Benzenesulphonic acid CAS 98-11-3				**p-Toluenesulphonic acid CAS 104-15-4**			
	Value	**Comment**	**KL.**	**Ref**	**Value**	**Comment**	**Kl.**	**Ref**
Melting point (°C)	50-51	anhydrous	4	1,2	106-107	anhydrous	2	1,2
Boiling point (°C)	319	calculated at 1013 hPa	2	3	140	@26.7 hPa	2	1
					332	calculated at 1013 hPa	2	3
Vapor pressure (hPa)	2.28E-05	calculated	2	3	3.9E-06	calculated	2	3
Partition coefficient (log K_{ow})	-1.17	calculated	2	3	-0.62	calculated	2	3
Water solubility (g/L at 25 °C)	689.5	calculated	2	3	202.3	calculated	2	3
					670	measured	2	2
					620	exp. database	2	3
Dissociation constant	0.7 at 25 °C		2	2				
(pKa)	-2.80	calculated	2	4	-2.58	calculated	2	4

Kl. = Klimisch criteria
Ref = Reference number

3.2. Environmental fate

The half-life for reaction with hydroxyl radicals in the atmosphere was estimated to be similar for both

substances. No hydrolysable groups are present in benzenesulphonic acid or p-toluenesulphonic acid. Distribution in the environment was calculated at Mackay Level III. If the sulphonic acids are released to the environment it will be to the water compartment (see table below). Including this in the program, both substances were found to stay in the water compartment.
No standard OECD301B or 301D microbial biodegradation studies are available on benzenesulphonic acid. Benzenesulphonic acid is reported to be biodegradable under aerobic conditions with adapted sludge, soil microorganisms or following MITI guidelines. The surrogate chemical p-toluenesulphonic acid was found to biodegrade for more than 90% in 5 days in two aerobic tests; it cannot be concluded that the surrogate is readily biodegradable because no standard, detailed described tests are available. In a study with adapted sludge (to each substance itself) both substances were degraded at the same rate (98.5% and 98.7% for benzene- and p-toluenesulphonic acid, respectively); the time elapsed is, however, not given. Based on the scientific literature it can be concluded by weight of the evidence that benzenesulphonic acid is biodegradable, but not whether the substance is readily biodegradable.

Conclusion: For all relevant endpoints on environmental fate, adequate data are available. The data available on biodegradation of both substances indicate that biodegradation is a pathway for removal from the environment. No further testing is recommended.

	Benzenesulphonic acid CAS 98-11-3				**p-Toluenesulphonic acid CAS 104-15-4**			
	Value	**Comment**	**KL.**	**Ref**	**Value**	**Comment**	**Kl.**	**Ref**
Photodegradation (t1/2)	19.2 days	calculated	2	3	7.8 days	calculated	2	3
Hydrolysis (t1/2)	-				-			
Distribution in water/air/soil/sediment	99.8/0.0/0.0/0.17%	calculated (emission to water only)	2	3	99.8/0.0/0.0/0.17%	calculated (emission to water only)	2	3
Biodegradability	degradable		4	6,7,18	degradable		4	14,18,19

Kl. = Klimisch criteria
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3.3. Ecotoxicity

For ecotoxicity no measured data are available for benzenesulphonic acid. For the surrogate, p-toluenesulphonic acid, an adequate acute fish study was reviewed that shows the absence of toxicity for aquatic species of this substance. The experimental result available for a daphnia acute study confirms this, but the actual conditions of this test cannot be verified. Since both substances have similar (calculated) physicochemical properties, experimental values for ecotoxicity studies for benzenesulphonic acid are expected to be also at a similar non-toxic level. Calculation of the relevant endpoints with the ECOSAR model confirms that benzenesulphonic acid and p-toluenesulphonic acid are not toxic for aquatic species. The calculated values do differ two to three orders of magnitude from the measured values for p-toluenesulphonic acid. Therefore, a daphnia test should be performed to confirm the validity of the surrogate's use for fish toxicity.

Conclusion: A daphnia test has to be performed to confirm that benzenesulphonic acid is not toxic to aquatic organisms. If the outcome of the test is positive, which is not expected, than also an algae test should be done to fulfill the HPV endpoints.

	Benzenesulphonic acid CAS 98-11-3				p-Toluenesulphonic acid CAS 104-15-4			
	Value	Comment	KL.	Ref	Value	Comment	Kl.	Ref
Acute fish (96-h LC50, mg/L)	1.12E06	calculated	4	3	>325		2	13
					3.71E05	calculated	4	3
Acute invertebrates (48-h EC50, mg/L)	9.63E05	calculated	4	3	>1625	exp. time not indicated	4	14
					3.31e05	calculated	4	3
Algal inhibition (96-h EC50, mg/L)	5.02E05	calculated	4	3	1.78E05	calculated	4	3

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3.4. Mammalian toxicity

Both substances are sulphonic acids, which are very acidic and therefore expected to show local effects in the gastrointestinal tract. The two substances have very similar dissociation constants (-2.8 and –2.58 for benzene- and p-toluenesulphonic acid, respectively). Therefore, absorption is expected to be comparable in the gastrointestinal tract.
Dermal absorption is expected to be low, because the partition coefficient is low.
p-Toluenesulphonic acid is classified as irritant to skin, eyes and inhalatory system (www.inchem.org). This is most likely due to the acidic nature of the molecule, which is similar for benzenesulphonic acid.

3.4.1. Acute toxicity

An oral LD50 value for rat is available for both substances. The values are very similar as expected. Thus this endpoint is covered sufficiently and the very reliable data for toxicity of p-toluenesulphonic acid can be used as a support for benzenesulphonic acid.

3.4.2. Genetic toxicity

An Ames test with a negative result is available for benzenesulphonic acid from a peer-reviewed article. For p-toluenesulphonic acid an adequate Ames test and chromosomal aberration test are available, both with a negative result. Because of the chemical similarity between these two compounds the results of the chromosomal aberration test for p-toluenesulphonic acid can be used as a surrogate for benzenesulphonic acid. Therefore this endpoint has been sufficiently investigated.

3.4.3. Repeated dose toxicity

No data are available in the public domain to satisfy this endpoint. Repeated dose toxicity can be considered a data gap. A 28-day repeated dose study must be performed.

3.4.4. Repro/developmental toxicity

No data are available on this endpoint, so a repro/developmental study should be performed.

Conclusion mammalian toxicity: Acute toxicity has been sufficiently investigated. For genetic toxicity adequate data are available. Repeated dose toxicity needs to be covered with a 28-day study. Repro/developmental toxicity needs to be investigated. Based on the data available this can most appropriately be executed in a combined study with repeated dose toxicity (OECD422).

	Benzenesulphonic acid CAS 98-11-3				p-Toluenesulphonic acid CAS 104-15-4			
	Value	**Comment**	**KL.**	**Ref**	**Value**	**Comment**	**Kl.**	**Ref**
Acute toxicity								
Acute oral (LD50, mg/kg)	1100	rat	2	11	1410	rat	1	15
Acute dermal (LD50, mg/kg)	-				-			
Acute inhalation (LC50, mg/m^3)	50% died in 14 days	8 h exposure; invalid study	3	11	-			
Genetic toxicity								
in vitro gene mutation (Ames test)	negative	no E.coli	2	12	negative	no E.coli	1	16
Chromosomal aberration	-				negative		1	17
Repeated dose	-				-			
Repro/developmental toxicity	-				-			

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3.5. SIDS Data matrix

Summary of the available data for all SIDS endpoints.

	Benzenesulphonic acid CAS 98-11-3				p-Toluenesulphonic acid CAS 104-15-4			
	Value	**Comment**	**KL.**	**Ref**	**Value**	**Comment**	**Kl.**	**Ref**
Physico-chemical								
Melting point (°C)	50-51	anhydrous	4	1,2	106-107	anhydrous	2	1,2
Boiling point (°C)	319	calculated at 1013 hPa	2	3	140	@26.7 hPa	2	1
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					670	measured	2	2
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Dissociation constant	0.7 at 25 °C		2	2				
(pKa)	-2.80	calculated	2	4	-2.58	calculated	2	4
Environmental fate								
Photodegradation (t1/2)	19.2 days	calculated	2	3	7.8 days	calculated	2	3
Hydrolysis (t1/2)	-				-			
Distribution in water/air/soil/sediment	99.8/0.0/0.0/0.17%	calculated (emission to water only)	2	3	99.8/0.0/0.0/0.17%	calculated (emission to water only)	2	3
Biodegradability	degradable		4	6,7, 18	degradable		4	14,18 ,19
Ecotoxicity								
Acute fish (96-h LC50, mg/L)	1.12E06	calculated	4	3	>325		2	13
					3.71E05	calculated	4	3
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Algal inhibition (96-h EC50, mg/L)	5.02E05	calculated	4	3	1.78E05	calculated	4	3
Mammalian toxicity								
Acute toxicity								
Acute oral (LD50, mg/kg)	1100	rat	2	11	1410	rat	1	15
Acute dermal (LD50, mg/kg)	-				-			
Acute inhalation (LC50, mg/m^3)	50% died in 14 days	8 h exposure; invalid study	3	11	-			
Genetic toxicity								
in vitro gene mutation (Ames test)	negative	no E.coli	2	12	negative	no E.coli	1	16
Chromosomal aberration	-				negative		1	17
Repeated dose	-				-			
Repro/developmental toxicity	-				-			

Kl. = Klimisch criteria, Ref = Reference number

4. Data availability and testing proposal

The availability of data is depicted in the following table. The study that should be performed to fill a data gap has been indicated.

	Benzenesulphonic acid CAS 98-11-3
Physico-chemical	
Melting point	+
Boiling point	+
Vapor Pressure	+
Partition Coefficient	+
Water Solubility	+
Environmental Fate	
Photodegradation	+
Hydrolysis	+
Distribution into compartments	+
Biodegradability	+
Ecotoxicity	
96-h LC50 Fish	+
48-h EC50 Daphnia	OECD202
72-h EC50 Algal Inhibition	+
Mammalian toxicity	
Acute	+
Repeated dose	OECD422
Genetic	+
Reproduction/developmental	OECD422

+ = data available
OECD = test to be performed

Adequate physicochemical and environmental data are available For ecotoxicity a daphnia test should be performed to confirm the non-toxicity concluded based on the present data. Genetic toxicity has been sufficiently investigated. For the data gaps in mammalian toxicity a combined test for repeated dose toxicity and reproduction/developmental toxicity screening is recommended.

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